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MATRIX ELEMENTS INCORPORATING MOMENTUM TRANSFER

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The theoretical calculations on electron capture phenomena in ion-atom collision at high energies, should include the translatory motion (momentum trans fer) of the electron attached either with the target or the projectile ion. Different authors viz. McCarroll, (1961) and Wilets *et al*, (1966) took recourse to approximate numerical analysis to evaluate the matrix elements $<\psi^n{}_A{}^*\,|\,V\,|\,\psi^m{}_B>$ and $<\psi^n{}_A{}^*\,\psi^m{}_B>$ occuring as coefficients in the set of differential equations to be solved cf. Basu *et al* (1967). But the difficulty is to call for the subroutine of the intergals at every step in the process of the solution of the differential equation (see Runge—Kutta Method). Cheshire (1967) has formulated a method in which the time derivatives of the said matrix elements can be found out analytically. He has pointed out how to calculate the matrix elements for 2s and 2p states. We had also pursued the problem with a straight forward alternative derivation and obtained results identical with those of Cheshire. Further the results have been utilised in calculating some of the matrix elements in alpha-hydrogen atom collision and proton-hydrogen atom collisions.

We write the hydrogenic wave functions (unnormalised) around two moving nuclei A and B as

$$\phi_{A,B} = \exp\Big[\; -\lambda_{A,B}r+i\,\mathbf{V}_{A,B}\cdot\mathbf{r}-\frac{i}{2}\,V^2{}_{A,B}\,t\;\; +\lambda_{A,}{}^2{}_B\,t\;\Big].$$

where $\mathbf{r}_A$, $\mathbf{r}_B$, $\mathbf{r}$ refer to the position vectors of the electron from nuclei A, B or any arbitrary origin 0, and $\mathbf{V}_A$, $\mathbf{V}_B$ the velocities of A and B. We note that

$$\mathbf{r}_{A,B}, = \mathbf{r}-\mathbf{V}_{A,B}\,t-\mathbf{S}_{A,B}$$

$$\mathbf{r} = \mathbf{V}_A-\mathbf{V}_B$$

$$\mathbf{r} = \mathbf{V}t+\mathbf{S}_A-\mathbf{S}_B.$$

We start with basic integral $I = \int \frac{\phi^*{}_A \phi_B}{r_A\, r_B}\, dv$

By using Fourier transform integral of $e^{\lambda R-}/R$ and writing in terms of r, we get

$$I = \frac{1}{4\pi^4} \exp\left[\frac{i}{2} t\, (V^2{}_A - V^2{}_B - \lambda^2{}_A + \lambda^2{}_B)\right] \times$$

$$\int \exp\, [i(\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{V}) \cdot \boldsymbol{r} - i\boldsymbol{p} \cdot (\boldsymbol{V}_A\, t + \boldsymbol{S}_B) - i\boldsymbol{q} \cdot (\boldsymbol{V}_B t + \boldsymbol{S}_B)] \times$$

$$\frac{1}{q^2+\lambda^2{}_B - p^2 - \lambda^2{}_A} \left[\frac{1}{p^2+\lambda^2{}_A} - \frac{1}{q^2+\lambda^2{}_B} \right] d^3r d^3p d^3q.$$

Now by using the Dirac δ-function, we have

$$I = \frac{2}{\pi} \exp\left[\frac{i}{2} t\, (V_A{}^2 - V_B{}^2 - \lambda_A{}^2 + \lambda_B{}^2)\right] \times$$

$$\int \exp[i\boldsymbol{q} \cdot (\boldsymbol{V}t + \boldsymbol{S}_A - \boldsymbol{S}_B)] \exp[-i\boldsymbol{V} \cdot (\boldsymbol{V}_A t + \boldsymbol{S}_B)] \times$$

$$\frac{1}{2\boldsymbol{q}.\boldsymbol{V} - V^2 - \lambda_A{}^2 + \lambda_B{}^2} \left[\frac{1}{|\boldsymbol{q}-\boldsymbol{V}|^2 + \lambda_A{}^2} - \frac{1}{q^2+\lambda_B{}^2} \right] d^3\boldsymbol{q}.$$

Taking time-derivative of I, the factor $(2\boldsymbol{q}.\boldsymbol{V} - V^2 - \lambda_A{}^2 + \lambda_B{}^2]$ cancels and using the relation $\frac{1}{2\pi^2} \int \frac{e^{i\boldsymbol{p}.\boldsymbol{r}}}{p^2+\lambda^2}\, d^3p = \frac{e^{-\lambda r}}{r}$, we get finally $i\frac{\partial I}{\partial t} = K(F-G)$,

where
$$K = \frac{2\pi}{R} \exp\left[i(\epsilon_B - \epsilon_A)t\right]$$

$$F = \exp\left[-\frac{i}{2} V^2 t - \lambda_B R - i\boldsymbol{V}.\boldsymbol{S}_A\right]$$

$$G = \exp\left[\frac{i}{2} V^2 t - \lambda_A R - i\boldsymbol{V}.\boldsymbol{S}_B\right].$$

Thus $I = -i \int K(F-G) dt$.

Differentiating I with respect to λ_A and λ_B several times-we can evaluate the general integrals of the type

$$\int r_A{}^m r_B{}^n \phi_A{}^* \phi_B dv = \left(-it\lambda_A - \frac{\partial}{\partial \lambda_A}\right)^{m+1} \left(it\lambda_B - \frac{\partial}{\partial \lambda_B}\right)^{n+1} I$$

If the general integrals involve θ and ϕ dependent wave functions in other than s-states, then we need to differentiate with respect to x, y or z component of S_A and S_B as necessary, in addition to the differentiations with respect to λ_A and λ_B.

Let us apply this technique in the calculation of the capture probabilities in the excited states of He^+ ion in α-particle-hydrogen atom collision. The matrix elements to be calculated by this method are

$$g_{mn} = \int \psi_m^* \psi'_n \, dv, \quad G_{mn} = \int \psi_m^* \frac{1}{2}\left(\frac{2}{r_B}+\frac{1}{r_A}\right) \psi'_n \, dv$$

where ψ_m is the wave function of H atom and ψ'_n that of He^+ ion.

Considering only the ground state of hydrogen atom the expressions for g_{1n} and G_{1n} are as following :

Taking $X = \frac{2\pi}{R} \exp\left[-2R+\frac{i}{2}(3-V^2)t\right]$

and $Y = \frac{2\pi}{R} \exp\left[-R+\frac{i}{2}(3+V^2)t\right]$,

$$g_{11} = \frac{2\sqrt{2}}{\pi}\Big[-2it^2\int (X-Y)dt+4it\int t(X-Y)dt-2i\int t^2(X-Y)dt-2t\int RYdt$$

$$+2\int tRYdt-t\int RXdt+\int tRXdt\Big]$$

$$G_{11} = \frac{\sqrt{2}}{\pi}\, i\left[2\int RYdt-\int RXdt\right]$$

Taking $M = \frac{2\pi}{R} \exp\left[-R-\frac{i}{2}V^2t\right]$ and $N = \frac{2\pi}{R}\exp\left[-R+\frac{i}{2}V^2t\right]$,

$$g_{12} = \frac{1}{\pi}\Big[-t^3\int (M-N)dt+3t^2\int t(M-N)dt-3t\int t^2(M-N)dt+\int t^3(M-N)dt$$

$$-2t\int RNdt+2\int tRNdt-t\int RMdt+\int tRMdt-\int tR^2Mdt+t\int R^2Mdt\Big]$$

$$+\frac{i}{\pi}\Big[-2t^2\int (M-N)dt+4t\int t(M-N)dt-2\int t^2(M-N)dt+t^2\int RNdt$$

$$-2t\int tRNdt+\int t^2RNdt+2t^2\int RMdt-4t\int tRMdt+2\int t^2RMdt\Big]$$

$$G_{12} = \frac{1}{\pi}\Big[t\int RNdt-\int t\,RNdt\Big]+\frac{i}{\pi}\Big[\int RNdt-\tfrac{1}{2}t^2\int Ndt+t\int tNdt-\tfrac{1}{2}\int t^2Ndt$$

$$-\tfrac{1}{2}\int RMdt+\tfrac{1}{2}t^2\int Mdt-t\int tMdt+\tfrac{1}{2}\,t^2Mdt+\tfrac{1}{2}\int R^2Mdt\Big]$$

$$g_{13} = \frac{V}{\pi}\Big[t^3 \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t(M-N)dt - 3t^2 \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^2(M-N)dt$$

$$+3t \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^3(M-N)dt - \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^4(M-N)dt - 2it^2 \int tMdt$$

$$-4it^2 \int tNdt + 4it \int t^2Mdt + 5it \int t^2Ndt - 2i \int t^3Mdt - 2i \int t^3Ndt$$

$$+it^3 \int Ndt - t^2 \int RNdt + 2t \int tRNdt - t \int tRMdt + \int t^2RMdt - \int t^2RNdt\Big]$$

$$G_{13} = \frac{V}{\pi}\Big[-\tfrac{1}{2}\, it^2 \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t(M-N)dt + i\,t \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^2(M-N)dt$$

$$-\tfrac{1}{2}\, i \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^3(M-N)dt - 2t \int tNdt + \tfrac{3}{2} \int t^2Ndt + \tfrac{1}{2}t^2 \int Ndt$$

$$-i \int tRNdt - \tfrac{1}{2} \int tRMdt + it \int RNdt\Big]$$

$$g_{14} = \frac{P}{\pi}\Big[t^3 \int \left(\frac{1}{R}+\frac{1}{R^2}\right)(M-N)dt - 3t^2 \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t(M-N)dt$$

$$+3t \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^2(M-Ndt - \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^3(M-N)dt - 2it^2 \int Mdt - it^2 \int Ndt$$

$$+4it \int tMdt + 2it \int tNdt - 2i \int t^2Mdt - i \int t^2Ndt - t \int RMdt + \int tRMdt\Big]$$

$$G_{14} = \frac{P}{\pi}\Big[-\tfrac{1}{2}\, it^2 \int \left(\frac{1}{R}+\frac{1}{R^2}\right)(M-N)dt + it \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t(M-N)dt$$

$$-\tfrac{1}{2}\, i \int \left(\frac{1}{R}+\frac{1}{R^2}\right) t^2(M-N)dt - t \int Ndt + \int tNdt - \tfrac{1}{2}\, i \int RMdt\Big]$$

$$g_{15} = G_{15} = 0.$$

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